Connecting via Winsock to STN

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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JUL 28	CA/CAplus patent coverage enhanced
NEWS	3	JUL 28	EPFULL enhanced with additional legal status information from the epoline Register
NEWS	4	JUL 28	IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS	5	JUL 28	STN Viewer performance improved
NEWS	6	AUG 01	INPADOCDB and INPAFAMDB coverage enhanced
NEWS	7	AUG 13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	8	AUG 15	CAOLD to be discontinued on December 31, 2008
NEWS	9	AUG 15	CAplus currency for Korean patents enhanced
NEWS	10	AUG 27	CAS definition of basic patents expanded to ensure comprehensive access to substance and sequence information
NEWS	11	SEP 18	Support for STN Express, Versions 6.01 and earlier, to be discontinued
NEWS	12	SEP 25	CA/CAplus current-awareness alert options enhanced to accommodate supplemental CAS indexing of exemplified prophetic substances
NEWS	13	SEP 26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS	14	SEP 29	IFICLS enhanced with new super search field
NEWS	15	SEP 29	EMBASE and EMBAL enhanced with new search and display fields
NEWS	16	SEP 30	CAS patent coverage enhanced to include exemplified prophetic substances identified in new Japanese-language patents
NEWS	17	OCT 07	EPFULL enhanced with full implementation of EPC2000
NEWS	18	OCT 07	Multiple databases enhanced for more flexible patent number searching
NEWS	19	OCT 22	Current-awareness alert (SDI) setup and editing enhanced
NEWS	20	OCT 22	WPIDS, WPINDEX, and WPIX enhanced with Canadian PCT Applications
NEWS	21	OCT 24	CHEMLIST enhanced with intermediate list of pre-registered REACH substances

NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items
NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:15:01 ON 29 OCT 2008

=> file registry

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.84	0.84

FILE 'REGISTRY' ENTERED AT 14:17:21 ON 29 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 OCT 2008 HIGHEST RN 1067631-14-4
DICTIONARY FILE UPDATES: 28 OCT 2008 HIGHEST RN 1067631-14-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH July 5, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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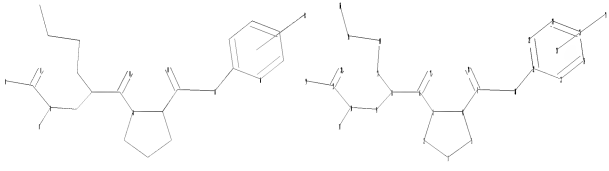
Uploading C:\Program Files\STNEXP\Queries\10527628.str



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1  2  3  4  5  22  23  24  25  26  27
chain bonds :
3-6  4-7  6-8  6-17  7-18  7-30  8-9  8-13  9-10  10-11  10-12  12-19  12-20  13-14
 14-15  15-16  22-30
ring bonds :
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exact/norm bonds :
2-3  3-4  3-6  6-17  7-18  7-30  9-10  10-11  10-12  12-20  22-30
exact bonds :
1-2  1-5  4-5  4-7  6-8  8-9  8-13  12-19  13-14  14-15  15-16
normalized bonds :
22-27  22-23  23-24  24-25  25-26  26-27
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS
10:CLASS  11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS
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L1      STRUCTURE UPLOADED

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=> d l1
L1 HAS NO ANSWERS
L1                STR
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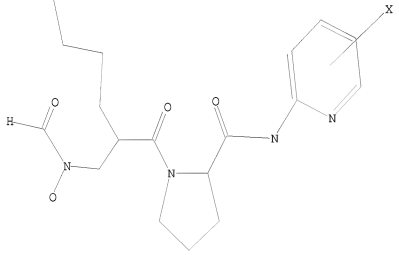


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Structure attributes must be viewed using STN Express query preparation.


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SAMPLE SEARCH INITIATED 14:33:10 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -       27 TO ITERATE

100.0% PROCESSED       27 ITERATIONS                              1 ANSWERS
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SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:           229 TO       851
PROJECTED ANSWERS:                1 TO        80

L2            1 SEA SSS SAM L1

=> s full l1
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FULL SCREEN SEARCH COMPLETED -      498 TO ITERATE

100.0% PROCESSED      498 ITERATIONS                                  16 ANSWERS
SEARCH TIME: 00.00.01

L3           16 SEA SSS FUL L1

=> d l3

L3   ANSWER 1 OF 16  REGISTRY  COPYRIGHT 2008 ACS on STN
RN   1056639-46-3  REGISTRY
ED   Entered STN:  03 Oct 2008
CN   INDEX NAME NOT YET ASSIGNED
FS   STEREOSEARCH
MF   C18 H24 F2 N4 O5
SR   CA
LC   STN Files:   CA, CAPLUS

Absolute stereochemistry.
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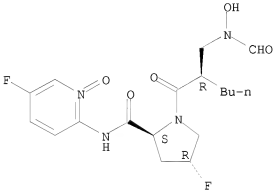


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**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

               1 REFERENCES IN FILE CA (1907 TO DATE)
               1 REFERENCES IN FILE CAPLUS (1907 TO DATE)


=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   193.70     194.54

FILE 'CAPLUS' ENTERED AT 14:35:03 ON 29 OCT 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 29 Oct 2008 VOL 149 ISS 18
FILE LAST UPDATED: 28 Oct 2008 (20081028/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html

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=> s l3/PREP
          36 L3
     4659780 PREP/RL
L4          8 L3/PREP
              (L3 (L) PREP/RL)

=> d ibib abs hitstr 1-8

L4   ANSWER 1 OF 8  CAPLUS  COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:         2007:1064533  CAPLUS
DOCUMENT NUMBER:          147:365790
TITLE:                    Preparation of N-formyl hydroxylamine proline
                          derivatives as peptidyl deformylase inhibitors
INVENTOR(S):              Lee, Kwangho; Leeds, Jennifer
PATENT ASSIGNEE(S):       Novartis AG, Switz.; Novartis Pharma GmbH
SOURCE:                   PCT Int. Appl., 63pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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     WO 2007106670        A2    20070920    WO 2007-US63167        20070302
     WO 2007106670        A3    20080124
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN,
             KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN,
             MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS,
             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF,
             BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW,
             GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
             BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA
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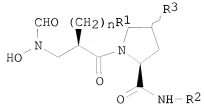
AU 2007226715	A1	20070920	AU 2007-226715			20070302
IN 2008DN07192	A	20081003	IN 2008-DN7192			20080822
PRIORITY APPLN. INFO.:			US 2006-779377P	P		20060303
			WO 2007-US63167	W		20070302

OTHER SOURCE(S): MARPAT 147:365790

GI



I

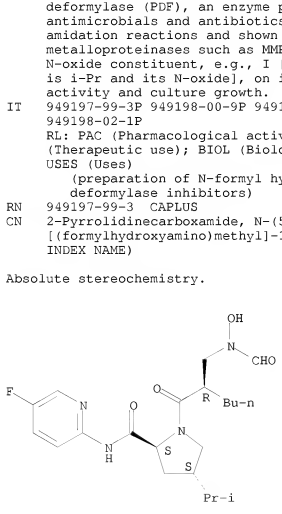
AB The invention relates to novel N-formyl hydroxylamine compds. I [R1 is H, alkyl, heteroalkyl, heterocycloalkyl, aryl, or heteroaryl; R2 is aryl or heteroaryl; R3 is alkyl or heteroalkyl; n is 0-3], which inhibit peptidyl deformylase (PDF), an enzyme present in prokaryotes, and are useful as antimicrobials and antibiotics. Compds. of the invention were prepared via amidation reactions and shown to be selective inhibitors of PDF vs. other metalloproteinases such as MMPs. A table shows the effect of P3 ring N-oxide constituent, e.g., I [(CH2)nR1 = Bu, R2 = 5-fluoro-2-pyridinyl, R3 is i-Pr and its N-oxide], on inhibition of Streptococcus pneumoniae PDF activity and culture growth.

IT 949197-99-3P 949198-00-9P 949198-01-0P
949198-02-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-formyl hydroxylamine proline derivs. as peptidyl deformylase inhibitors)

RN 949197-99-3 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-4-(1-methylethyl)-, (2S,4S)- (CA INDEX NAME)

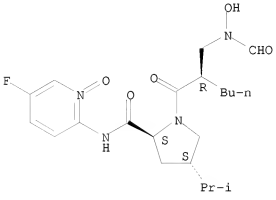
Absolute stereochemistry.



RN 949198-00-9 CAPLUS

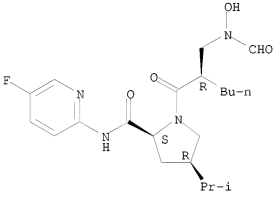
CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-4-(1-methylethyl)-, (2S,4S)- (CA INDEX NAME)

Absolute stereochemistry.



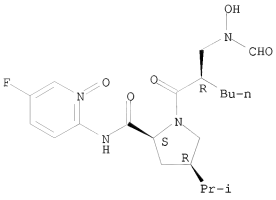
RN 949198-01-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-4-(1-methylethyl)-, (2S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 949198-02-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-4-(1-methylethyl)-, (2S,4R)- (CA INDEX NAME)

Absolute stereochemistry.

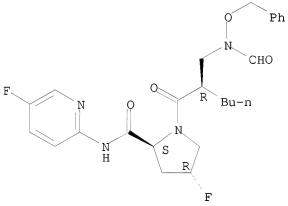


IT 915280-68-1P 915280-69-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-formyl hydroxylamine proline derivs. as peptidyl deformylase inhibitors)

RN 915280-68-1 CAPLUS

CN 2-Pyrrolidinecarboxamide, 4-fluoro-N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S,4R)- (CA INDEX NAME)

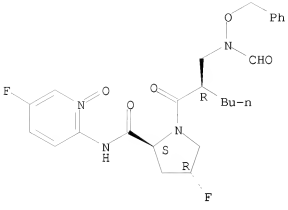
Absolute stereochemistry.



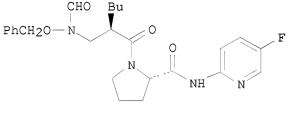
RN 915280-69-2 CAPLUS

CN 2-Pyrrolidinecarboxamide, 4-fluoro-N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1263091 CAPLUS
DOCUMENT NUMBER: 146:184267
TITLE: β-Amino amides from β-lactams: application to the formal synthesis of a peptide-deformylase inhibitor
AUTHOR(S): Jiang, Xinglong; Prasad, Kapa; Prashad, Mahavir; Slade, Joel; Repic, Oljan; Blacklock, Thomas J.
CORPORATE SOURCE: Process Research & Development, Novartis Pharmaceuticals Corporation, East Hanover, NJ, 07936, USA
SOURCE: Synlett (2006), (18), 3179-3181
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:184267
GI



I

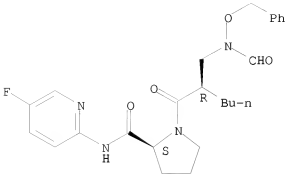
AB A facile and a practical synthesis of I, an intermediate for a peptide-deformylase inhibitor, is described using an acid-catalyzed aminolysis of a β-lactam with a pyrrolidine derivative as the key transformation. In addition, simplified conditions for the conversion of a β-hydroxy acid to a β-lactam are reported.

IT 478913-92-7P 771478-83-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(formal synthesis of peptide-deformylase inhibitor via aminolysis of β-lactam)

RN 478913-92-7 CAPLUS

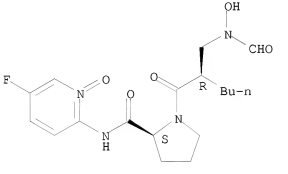
CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-(phenylmethoxy)-β-alanyl-N-(5-fluoro-2-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 771478-83-2 CAPLUS
CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-hydroxy-β-alanyl-N-(5-fluoro-1-oxido-2-pyridinyl)-, magnesium salt (2:1) (CA INDEX NAME)

Absolute stereochemistry.



●1/2 Mg

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:1250645 CAPLUS
DOCUMENT NUMBER: 146:45733
TITLE: Preparation of N-formylhydroxylamine-containing peptides
INVENTOR(S): Bracken, Kathryn Rene; Bushell, Simon; Dean, Karl; Francavilla, Charles; Jain, Rakesh K.; Lee, Kwangho; Seepersaud, Mohindra; Shu, Lei; Sundaram, Arathia; Yuan, Zhengyu
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.; Vicuron Pharmaceuticals, Inc
SOURCE: PCT Int. Appl., 61pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2006127576 A2 20061130 WO 2006-US19688 20060522
WO 2006127576 A3 20070125
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
AU 2006251612 A1 20061130 AU 2006-251612 20060522
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IN 2007DN08662 A 20071214 IN 2007-DN8662 20071108
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KR 2008015411 A 20080219 KR 2007-727226 20071122
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OTHER SOURCE(S): MARPAT 146:45733
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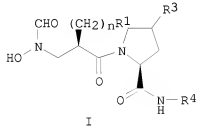


I

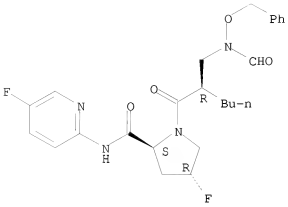
AB The invention relates to novel N-formyl hydroxylamine compds. I (R1 is H, alkyl, heteroalkyl, heterocycloalkyl, aryl, or heteroaryl; R3 is H, halo, or alkoxy; R4 is aryl or heteroaryl; n is 0-3) or their salts or prodrugs that inhibit peptidyl deformylase (PDF), an enzyme present in prokaryotes, and are useful as antimicrobials and antibiotics. Examples describe syntheses of title compds. and intermediates, e.g., for the preparation of I (n = 1, R1 = cyclopentyl, R3 =s H, R4 = 5-fluoro-N-oxido-2-pyridyl). Compds. of the invention were assayed for inhibition of PDF and for antimicrobial activity (e.g., min. inhibitory concns. .apprx. 0.25-32 μg/mL against H. influenza).

IT 915280-68-1P 915280-69-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-formylhydroxylamine-containing peptides as inhibitors of peptidyl deformylase)

RN 915280-68-1 CAPLUS

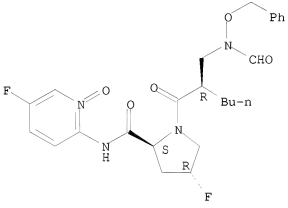
CN 2-Pyrrolidinecarboxamide, 4-fluoro-N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



RN 915280-69-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-fluoro-N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S,4R)- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:14391 CAPLUS
DOCUMENT NUMBER: 142:113909
TITLE: Process for preparation of N-[oxidopyridinyl) L-prolinamide derivatives
INVENTOR(S): Slade, Joel; Vivelo, James Anthony; Chen, Guang-Pei; Bajwa, Joginder Singh; Parker, David John
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005000835	A1	20050106	WO 2004-EP6915	20040625
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
SN, TD, TG

AU 2004251876	A1	20050106	AU 2004-251876		20040625
CA 2530142	A1	20050106	CA 2004-2530142		20040625
EP 1641778	A1	20060405	EP 2004-740324		20040625
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK					
BR 2004011921	A	20060815	BR 2004-11921		20040625
CN 1829710	A	20060906	CN 2004-80021438		20040625
MX 2005PA14217	A	20060309	MX 2005-PA14217		20051221
US 20070060753	A1	20070315	US 2005-561754		20051221
IN 2005CN03523	A	20070831	IN 2005-CN3523		20051226
PRIORITY APPLN. INFO.:			US 2003-482686P	P	20030626
			WO 2004-EP6915	W	20040625

OTHER SOURCE(S): CASREACT 142:113909; MARPAT 142:113909

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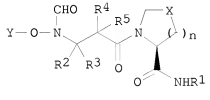

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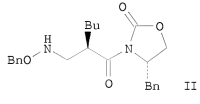

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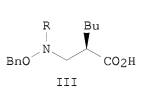

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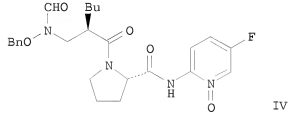


IV

AB A process for the preparation of title compds. of formula I [Y = a OH protecting group; R1 =(hetero)aryl; R2-R5 = independently H or alkyl, or R2R3 and/or R4R5 = cycloalkyl; X = CH2, S, CH(OH), etc.; n = 0-3] is disclosed. For example, contacting II•TsOH with 1N Na2CO3 in EtOAc to move TsOH and oxidation by H2O2 gave III (R = H). Formylation of III with formic acetic anhydride gave III (R = CHO). Reaction of III with HBr salt of N-(5-fluoro-2-pyridinyl)-2-pyrrolidinecarboxamide, followed by oxidation , gave IV. Thus, the present invention provides a process producing the title compound, which are useful to prepare certain antibacterial N-formyl hydroxylamine compds. as peptide deformylase inhibitors.

IT 478913-92-7P

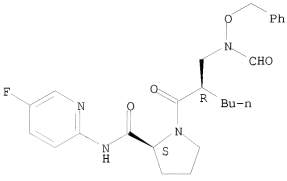
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-[oxidopyridinyl) L-prolinamide derivs.)

RN 478913-92-7 CAPLUS

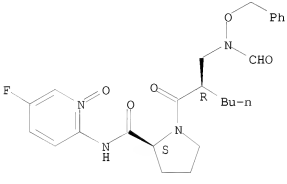
CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-(phenylmethoxy)-β-alanyl-N-(5-fluoro-2-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 478913-93-8P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of N-[oxidopyridinyl) L-prolinamide derivs.)
RN 478913-93-8 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:857380 CAPLUS
DOCUMENT NUMBER: 141:337761
TITLE: Crystalline N-formylhydroxylamine compounds for pharmaceuticals
INVENTOR(S): Mueller, Martin; Liu, Hui; Bajwa, Joginder Singh
PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH; Slade, Joel
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004087133	A1	20041014	WO 2004-EP3478	20040401
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,				

GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG

AU 2004226815	A1	20041014	AU 2004-226815		20040401
AU 2004226815	B2	20070719			
CA 2520682	A1	20041014	CA 2004-2520682		20040401
EP 1613305	A1	20060111	EP 2004-725014		20040401
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
BR 2004009009	A	20060328	BR 2004-9009		20040401
CN 1764450	A	20060426	CN 2004-80007872		20040401
JP 2006522054	T	20060928	JP 2006-504952		20040401
US 20070135353	A1	20070614	US 2004-550631		20040401
ZA 2005007179	A	20060426	ZA 2005-7179		20050907
IN 2005CN02467	A	20070831	IN 2005-CN2467		20050930
NO 2005005097	A	20051222	NO 2005-5097		20051101
PRIORITY APPLN. INFO.:			US 2003-459726P	P	20030402
			WO 2004-EP3478	A	20040401

OTHER SOURCE(S): MARPAT 141:337761

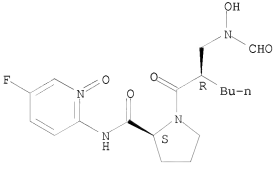
AB Certain N-formylhydroxylamine compds., such as N-[1-oxo-2-alkyl-3-(N-hydroxyformamido)propyl](carbonylaminoaryl)azacycloalkanes are useful in the treatment of bacterial infections. Disclosed are crystalline salts of such compds. Thus, a capsule contained a N-formylhydroxylamine 200, spray-dried lactose 148, and Mg stearate 2 mg. 1-{2-R-[(formylhydroxylamino)methyl]hexanoyl}pyrrolidone-2S-carboxylic acid-(4-ethylpyridin-2-yl)amide was converted to its calcium salt by reaction with CaCl2 solution in NaOH solution

IT 771478-83-2P
RL: PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystalline N-formylhydroxylamine compds. for pharmaceuticals)

RN 771478-83-2 CAPLUS

CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-hydroxy-β-alanyl-N-(5-fluoro-1-oxido-2-pyridinyl)-, magnesium salt (2:1) (CA INDEX NAME)

Absolute stereochemistry.



●1/2 Mg

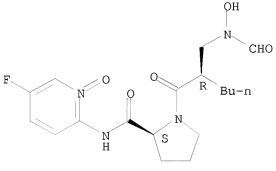
IT 771478-84-3P 771478-85-4P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(crystalline N-formylhydroxylamine compds. for pharmaceuticals)

RN 771478-84-3 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-, zinc salt (2:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.

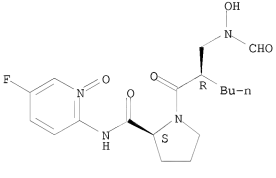


●1/2 Zn

RN 771478-85-4 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-, calcium salt (2:1), (2S)- (CA INDEX NAME)

Absolute stereochemistry.



●1/2 Ca

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:740215 CAPLUS

DOCUMENT NUMBER: 141:261060

TITLE: Process for preparing β-amino acid intermediates in the synthesis of aminoacylpyrrolidinecarboxamides and related antibacterial compounds

INVENTOR(S): Prashad, Mahavir; Kim, Hang-yong; Hu, Bin; Slade, Joel; Kapa, Prasad Koteswara; Girgis, Michael John
PATENT ASSIGNEE(S): Novartis Ag, Switz.; Novartis Pharma GmbH
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004076053	A2	20040910	WO 2004-US5159	20040220
WO 2004076053	A3	20041202		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004216178	A1	20040910	AU 2004-216178	20040220
AU 2004216178	B2	20080703		
CA 2516465	A1	20040910	CA 2004-2516465	20040220
EP 1599440	A2	20051130	EP 2004-713381	20040220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007448	A	20060131	BR 2004-7448	20040220
CN 1759097	A	20060412	CN 2004-80006326	20040220
JP 2006519786	T	20060831	JP 2006-503764	20040220
CN 101092342	A	20071226	CN 2007-10136131	20040220
IN 2005CN01956	A	20070831	IN 2005-CN1956	20050818
MX 2005PA08842	A	20051005	MX 2005-PA8842	20050819
US 20070179298	A1	20070802	US 2007-544919	20070424

PRIORITY APPLN. INFO.:		
US 2003-449015P	P	20030221
US 2003-449016P	P	20030221
US 2003-449017P	P	20030221
CN 2004-80006326	A3	20040220
WO 2004-US5159	A	20040220

OTHER SOURCE(S): CASREACT 141:261060; MARPAT 141:261060
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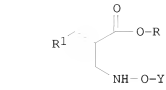

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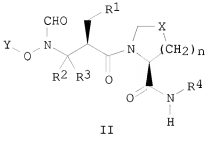


II

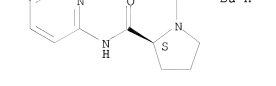
AB β-Amino acid derivs. I (R is alkyl, R1-R3 are H or alkyl or R2R3C are cycloalkyl, Y is a protecting group), intermediates in the synthesis of aminoacyl azacycloalkanes II [same R-R3 and Y, R4 is aryl or heteroaryl, n is 0-3, X is CH2, S, CHOH, CH(OR), CH(SH), CF2, C:N(OR) or CHF] were prepared by hydrogenation of corresponding α-alkylidene derivs. in the presence of a chiral ligand and a catalytic amount of a hydrogenation catalyst. Thus, a mixture of 2-[[(phenylmethoxy)amino]methyl]-2-hexenoic acid Me ester (.apprx. 1:1 E/Z, preparation given), bis(norbornadiene)rhodium(I) tetrafluoroborate and (1S,1'S,2R,2'R)-TangPhos in deoxygenated methanol in a Parr bottle is hydrogenated under H2 (45-55 psi) at room temperature for 24 h to afford 94 % 2-[[(phenylmethoxy)amino]methyl]-(2S)-hexanoic acid Me in 95 % yield (R:S = 98:2).

IT 478912-56-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of β-amino acid intermediates in synthesis of aminoacylpyrrolidinecarboxamides and related antibacterial compds.)

RN 478912-56-0 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:267293 CAPLUS

DOCUMENT NUMBER: 140:287275
TITLE: Process for preparing benzyloxyaminoacylpyrrolidinecarboxamides
INVENTOR(S): Kapa, Prasad Koteswara; Jiang, Xinglong; Loeser, Eric M.; Slade, Joel; Prashad, Mahavir; Lee, George Tien-San
PATENT ASSIGNEE(S): Novartis A.-G., Switz.; Novartis Pharma G.m.b.H.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004026824	A1	20040401	WO 2003-EP10416	20030918
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SE, SG, SK, SY, TJ, TM, TN, TR, TT, UA, US, UZ, VC, VN, YU, ZA, ZW				
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR				
CA 2499426	A1	20040401	CA 2003-2499426	20030918
AU 2003273404	A1	20040408	AU 2003-273404	20030918
AU 2003273404	B2	20080522		
EP 1542968	A1	20050622	EP 2003-755559	20030918
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003014592	A	20050809	BR 2003-14592	20030918
CN 1684945	A	20051019	CN 2003-822471	20030918
JP 2006503053	T	20060126	JP 2004-537129	20030918
NZ 538833	A	20080530	NZ 2003-538833	20030918
ZA 2005001923	A	20050912	ZA 2005-1923	20050307
IN 2005CN00346	A	20070406	IN 2005-CN346	20050308
MX 2005PA03089	A	20050527	MX 2005-PA3089	20050318
NO 2005001867	A	20050418	NO 2005-1867	20050418
US 20050261504	A1	20051124	US 2005-527628	20050525

PRIORITY APPLN. INFO.:	US 2002-411920P	P	20020919
	US 2003-480242P	P	20030620
	WO 2003-EP10416	W	20030918

OTHER SOURCE(S): CASREACT 140:287275; MARPAT 140:287275
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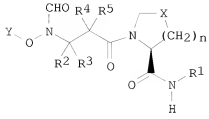

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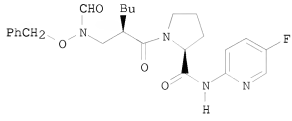


II

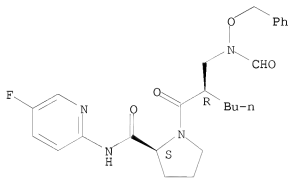
AB Title compds. I [Y = protective group; R1 = aryl, heteroaryl; R2-R5 = H, aliph; R2R3, R4R5 = alkylene; X = CH2, S, (un)substituted CH(OH), CH(SH), CF2, C:NOH, CHF; n = 0-3] were prepared for use as intermediates to prepare certain antibacterial N-formyl hydroxylamine compds. which are peptide deformylase inhibitors. Thus, HOCH2CHBuCO2H was treated with PhCH2ONH2, followed by MeSO2Cl to give MeSO3CH2CHBuCONHOCH2Ph, which was cyclized to the β-lactam and treated with (S)-N-(5-fluoro-2-pyridinyl)pyrrolidine-2-carboxamide, followed by formylation to give the pyrrolidine II.

IT 478913-92-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process for preparing benzyloxyaminoacylpyrrolidinecarboxamides)

RN 478913-92-7 CAPLUS

CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-(phenylmethoxy)-β-alanyl-N-(5-fluoro-2-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2002:977804 CAPLUS
DOCUMENT NUMBER: 138:55863
TITLE: Preparation of N-formyl-N-hydroxylamino-substituted pyrrolidine derivatives as inhibitors of peptidyl

deformylase

INVENTOR(S): Patel, Dinesh V.; Yuan, Zhengyu; Jain, Rakesh K.; Garcia Alvarez, Salvador; Jacobs, Jeffrey

PATENT ASSIGNEE(S): Versicor, Inc., USA; Novartis AG

SOURCE: PCT Int. Appl., 69 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

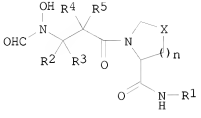
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002102790	A1	20021227	WO 2002-EP6604	20020614
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LT, LU, LV, MA, MD, MK, MN, MX, NO, NZ, OM, PH, PL, PT, RO, RU, SE, SG, SI, SK, TJ, TM, TN, TR, TT, UA, US, UZ, VN, YU, ZA, ZW				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2448526	A1	20021227	CA 2002-2448526	20020614
AU 2002321062	A1	20030102	AU 2002-321062	20020614
AU 2002321062	B2	20060202		
US 20030045479	A1	20030306	US 2002-171706	20020614
US 7148242	B2	20061212		
EP 1401828	A1	20040331	EP 2002-754681	20020614
EP 1401828	B1	20060412		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
HU 2004000208	A2	20040628	HU 2004-208	20020614
CN 1511152	A	20040707	CN 2002-810596	20020614
BR 2002010377	A	20040810	BR 2002-10377	20020614
JP 2005502606	T	20050127	JP 2003-506263	20020614
NZ 529489	A	20051028	NZ 2002-529489	20020614
AT 323081	T	20060415	AT 2002-754681	20020614
PT 1401828	T	20060831	PT 2002-754681	20020614
ES 2262824	T3	20061201	ES 2002-754681	20020614
RU 2325386	C2	20080527	RU 2003-137565	20020614
ZA 2003008379	A	20040521	ZA 2003-8379	20031028
IN 2003CN01963	A	20060106	IN 2003-CN1963	20031210
NO 2003005571	A	20040216	NO 2003-5571	20031212
MX 2003PA11628	A	20050307	MX 2003-PA11628	20031215
HK 1064370	A1	20061020	HK 2004-107013	20040914

PRIORITY APPLN. INFO.:	US 2001-298419P	P	20010615
	US 2002-360313P	P	20020227
	WO 2002-EP6604	W	20020614

OTHER SOURCE(S): MARPAT 138:55863

GI



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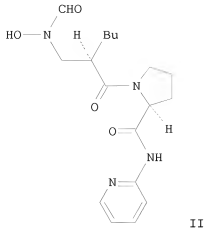


II

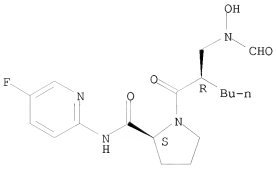
AB Title compds. I [X = CH2, S, CHOH, CH-alkoxy, CHSH, etc.; R1 = (hetero)aryl; R2-5 = H, alkyl, etc.; n = 0-3 provided that when n = 0, X = CH2] are prepared For instance, (S)-2-(chlorocarbonyl)pyrrolidine-1-carboxylic acid benzyl ester is used to acylate 2-aminopyridine and the resulting amide deprotected and coupled to (2R)-2-[(benzyloxyformylamino)methyl]hexanoic acid (preparation given; dioxane, HATU, i-Pr2NEt) to give II. IC50 of selected examples of I against MMP-7 ranges from >10 pM to >100 pM, whereas the IC50 of these same compds. against zinc-containing peptidyl deformylase (PDF) ranges from about 0.005 pM to 5 pM, and against nickel-containing PDF ranges from about 0.001 pM to about 0.3 pM. I are useful for preventing contamination of a cell culture medium.

IT 478912-56-0P, (2S)-1-[(2R)-2-[(Formylhydroxyamino)methyl]hexanoyl]pyrrolidine-2-carboxylic acid N-(5-fluoropyridin-2-yl)amide 478912-69-5P, (2S)-1-[(2R)-2-[(Formylhydroxyamino)methyl]hexanoyl]pyrrolidine-2-carboxylic acid N-(6-fluoropyridin-2-yl)amide 478913-91-6P, (2S)-1-[(2R)-2-[(Formylhydroxyamino)methyl]hexanoyl]pyrrolidine-2-carboxylic acid N-(5-fluoro-1-oxopyridin-2-yl)amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-formyl-N-hydroxylamino-substituted pyrrolidine derivs. as inhibitors of peptidyl deformylase)

RN 478912-56-0 CAPLUS

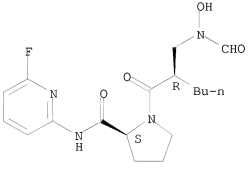
CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



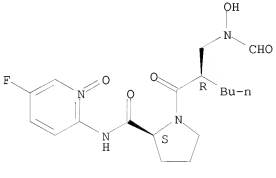
RN 478912-69-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, N-(6-fluoro-2-pyridinyl)-1-[(2R)-2-[(formylhydroxyamino)methyl]-1-oxohexyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 478913-91-6 CAPLUS
CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-hydroxy-β-alanyl-N-(5-fluoro-1-oxido-2-pyridinyl)- (CA INDEX NAME)

Absolute stereochemistry.



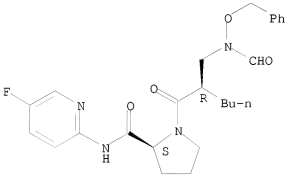
IT 478913-92-7P, (2S)-1-[(2R)-2-[(Benzyloxyformylamino)methyl]hexanoyl]pyrrolidine-2-carboxylic acid N-(5-fluoropyridin-2-yl)amide 478913-93-8P, (2S)-1-[(2R)-2-[(Benzyloxyformylamino)methyl]hexanoyl]pyrrolidine-2-carboxylic acid N-(5-fluoro-1-oxopyridin-2-yl)amide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-formyl-N-hydroxylamino-substituted pyrrolidine derivs. as inhibitors of peptidyl deformylase)

RN 478913-92-7 CAPLUS

CN L-Prolinamide, (2R)-2-butyl-N-formyl-N-(phenylmethoxy)-β-alanyl-N-(5-fluoro-2-pyridinyl)- (CA INDEX NAME)

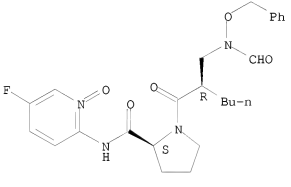
Absolute stereochemistry. Rotation (-).



RN 478913-93-8 CAPLUS

CN 2-Pyrrolidinecarboxamide, N-(5-fluoro-1-oxido-2-pyridinyl)-1-[(2R)-2-[[formyl(phenylmethoxy)amino]methyl]-1-oxohexyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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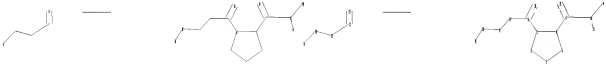
Uploading C:\Program Files\STNEXP\Queries\10527628B.str



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chain nodes :
6  7  8  9  10  11  12  13  15  16  19  20  21  22  23  24
ring nodes :
1  2  3  4  5
chain bonds :
3-6  4-7  6-8  6-12  7-13  7-16  8-9  9-10  10-11  15-16  16-24  19-20  20-21
21-22  22-23
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
2-3  3-4  3-6  6-12  7-13  7-16  9-10  10-11  15-16  19-20  22-23
exact bonds :
1-2  1-5  4-5  4-7  6-8  8-9  16-24  20-21  21-22
isolated ring systems :
containing 1 :


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS
10:CLASS  11:CLASS  12:CLASS  13:CLASS  15:Atom  16:CLASS  19:CLASS  20:CLASS
21:CLASS  22:CLASS  23:CLASS  24:CLASS
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 19



L5      STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5              STR

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.


=> s sam l5
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE
COMMAND STACK INTERRUPTED.  ENTER "DISPLAY HISTORY"
TO SEE WHICH COMMANDS WERE EXECUTED.


=>
=> s sam l5
   REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.
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MULTIPLE ROLE QUERIES ARE NOT ALLOWED IN A NON-REACTION FILE
COMMAND STACK INTERRUPTED.  ENTER "DISPLAY HISTORY"
TO SEE WHICH COMMANDS WERE EXECUTED.


=>
=> file casreact
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.48     286.30

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                     0.00      -6.40

FILE 'CASREACT' ENTERED AT 15:30:56 ON 29 OCT 2008
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FILE CONTENT:1840 - 25 Oct 2008 VOL 149 ISS 18

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************************************************************
*                                                          *
*     CASREACT now has more than 15.3 million reactions    *
*                                                          *
************************************************************

CASREACT contains reactions from CAS and from: ZIC/VINITI database
(1974-1999) provided by InfoChem; INPI data prior to 1986;
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This file contains CAS Registry Numbers for easy and accurate substance
identification.

=> s sam l5
SAMPLE SEARCH INITIATED 15:31:02 FILE 'CASREACT'
SCREENING COMPLETE -        0 REACTIONS TO VERIFY FROM         0 DOCUMENTS

100.0% DONE       0 VERIFIED       0 HIT RXNS                        0 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:         0 TO        0
PROJECTED ANSWERS:               0 TO        0

L6            0 SEA SSS SAM L5 (     0 REACTIONS)

=> s full l5
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FULL SEARCH INITIATED 15:31:12 FILE 'CASREACT'
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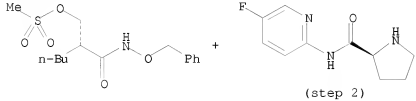
100.0% DONE 48 VERIFIED 40 HIT RXNS 3 DOCS
SEARCH TIME: 00.00.02

L7 3 SEA SSS FUL L5 (40 REACTIONS)

=> d l7

L7 ANSWER 1 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(8) OF 15 - 2 STEPS



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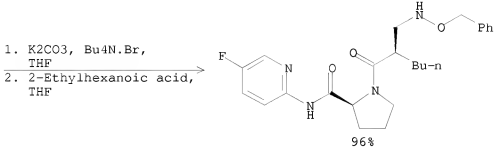

96%

REF: Synlett, (18), 3179-3181; 2006
CON: STEP(1) 6 hours, 40 deg C
STEP(2) 7 hours, 72 deg C

=> d ibib abs hitstr 1-3
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

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SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path".  Displays all single step reactions which
             contain a hit substance.  Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes.  For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>).  Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD.  The information is displayed in the same order
as the specification.  All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):fcrdref

L7   ANSWER 1 OF 3  CASREACT  COPYRIGHT 2008 ACS on STN
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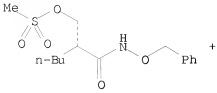
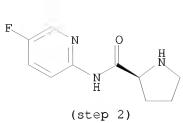
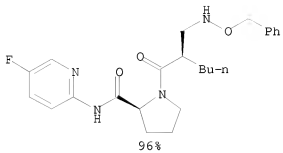
RX(8) OF 15 - 2 STEPS





(step 2)

1. K2CO3, Bu4N.Br, THF
2. 2-Ethylhexanoic acid, THF

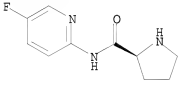


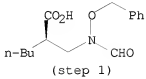
96%

REF: Synlett, (18), 3179-3181; 2006
CON: STEP(1) 6 hours, 40 deg C
STEP(2) 7 hours, 72 deg C

L7 ANSWER 2 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(3) OF 10

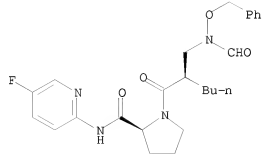




(step 1)

2 HBr
(step 2)

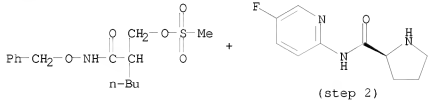
1. Dicyclohexylamine, Citric acid, AcOEt, Water
2. EDAP, 1-Benzotriazolol, N-Methylmorpholine, Water

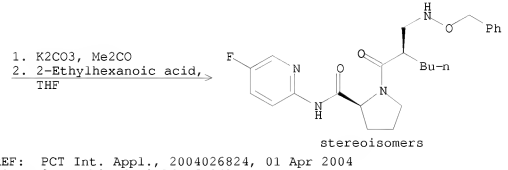


REF: PCT Int. Appl., 2005000835, 06 Jan 2005
CON: STAGE(1) room temperature; 10 minutes, room temperature
STAGE(2) room temperature; room temperature -> 5 deg C;
room temperature; overnight

L7 ANSWER 3 OF 3 CASREACT COPYRIGHT 2008 ACS on STN

RX(16) OF 57 - 2 STEPS





REF: PCT Int. Appl., 2004026824, 01 Apr 2004
NOTE: 2) combined yield of 84%
CON: STEP(1.1) room temperature -> reflux; 30 minutes, reflux; 1 hour,
reflux
STEP(2) 7 hours, room temperature -> 70 deg C

=>
=> exit
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF
LOGOFF? (Y)/N/HOLD:y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	147.74	434.04
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-6.40

STN INTERNATIONAL LOGOFF AT 15:54:47 ON 29 OCT 2008